

Photoemission Fermi Surface Topology Studies of Magnetic Alloys

M. Hochstrasser¹, R.F. Willis¹, F.O. Schumann², J.G. Tobin², and Eli Rotenberg³

¹The Pennsylvania State University, University Park, State College, Pennsylvania 16802, USA

²Lawrence Livermore National Laboratory, University of California, Livermore, California 94550, USA

³Advanced Light Source, Ernest Orlando Lawrence Berkeley National Laboratory,
University of California, Berkeley, California 94720, USA

ABSTRACT

Cuts through the Fermi Surfaces of CoNi and FeNi alloy films epitaxially grown on fcc Cu(100) reveal topological features in angle-resolved photoemission. Changing the stoichiometry of these pseudomorphic films permits us to observe changes in the Fermi surfaces. Increasing Co or Fe content, increases the ferromagnetism from that of pure Ni. The average moment increases linearly in the case of CoNi alloys but is arrested and sharply declines in FeNi. This work attempts to identify the electronic features underpinning this difference.

INTRODUCTION

Measurements with the surface magneto-optic Kerr effect (SMOKE) and magnetic dichroism of the Fe, Co, and Ni 3p core levels in photoemission with linearly polarized light (XMLD) have shown that the elemental moments remain constant and finite, while the magnetization increases with increasing Co and Fe content [1]. In the FeNi alloys, this linear increase of the average magnetic moment, shows a sharp decrease for richer Fe concentrations [2]. Mössbauer spectroscopy and SQUID magnetometry have shown that in the Fe-rich FeNi alloys an antiferromagnetic phase emerges, which coexists with the ferromagnetic phase [3]. It is this 'mixed' phase, rather than any collapse in the magnitude of the magnetic moments that is, believed to be responsible for the observed decrease in the ferromagnetic order.

RESULTS AND DISCUSSION

States at the Fermi energy are recorded in the high symmetrical k-plane for films 8 ML thick to avoid any contribution from the Cu substrate. Patterns 1(a), (b), (c) and (d) show data for a (110) cut through Brillouin zone in extended k-space. The alloy concentrations are from left to right: pure Co (a), Co₆₀Ni₄₀ (b), Co₄₀Ni₆₀ (c), pure Ni (d). In this (110) plane, one feature remains characteristic of the whole concentration range and sharply defined. It connects the L points in the fcc Brillouin zone more or less continuously throughout momentum space. This feature is due to the sp band and forms a 'dogbone' hole pocket, similar to that in copper.

As the number of holes in the alloy increases going from pure Ni towards pure Co, emission from new states occurs at the center of the zone as well as across the neck of this 'dogbone' structure. In simple terms, with increasing Co concentration the Fermi level shifts to lower energies and cuts through the d-band in the center of the zone near the Γ point, as suggested by the pseudomorphic bandstructures of Cu, Ni, Co, and Fe [4]. Also with increasing Co concentration, the exchange splitting of the minority and majority d-bands increases in a way that would indicate that this intensity surrounding the zone center is due mainly to minority spin polarized d-states. The 'dogbone' structure, a characteristic feature due to the sp-band collects some d-character but does not change dramatically. This 'dogbone' is a characteristic feature of these fcc 3d materials. Across the neck of this dogbone an increase of intensity is observed with increasing number of holes suggesting increasing hybridization with the sp-band close to the Fermi level in this particular region of k-space. This enhances electron scattering between d and sp-states.

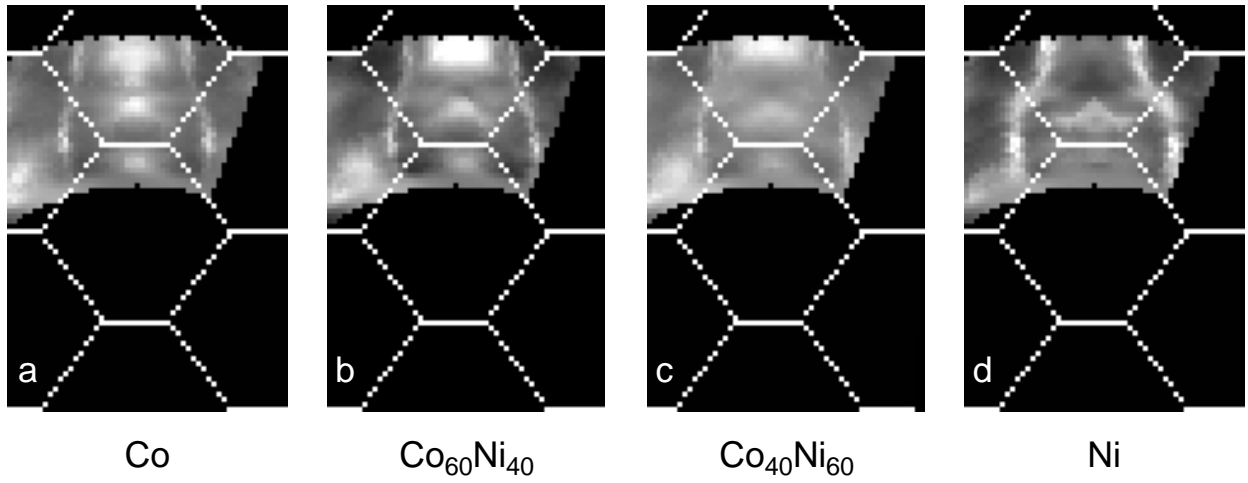


Figure 1. Fermi contour maps in the [110] plane obtained in the photon energy range between 80 eV and 195 eV of a pure fcc Co film (a) fcc alloy films $\text{Co}_{60}\text{Ni}_{40}$ (b), fcc $\text{Co}_{40}\text{Ni}_{60}$ (c), and a pure fcc Ni film (d), all grown epitaxially on Cu(100).

The FeNi alloys show a similar evolution of states at the Fermi energy with increasing Fe content. Again, we observe a strong contribution due to the sp-band and a clearly defined 'dogbone' feature. Enhanced intensity in the center of the Brillouin zone and across the neck of this dogbone again appears with increased emptying of the d-bands. We observe well defined states in this momentum space, which is a strong indication that the muffin-tin potential on the different atomic sites, Fe, Ni, respectively Co is very similar. Any increased diffuseness in the patterns appears mainly in the d-states, which is expected since the lifetimes of these states is less due to increased scattering out of these states.

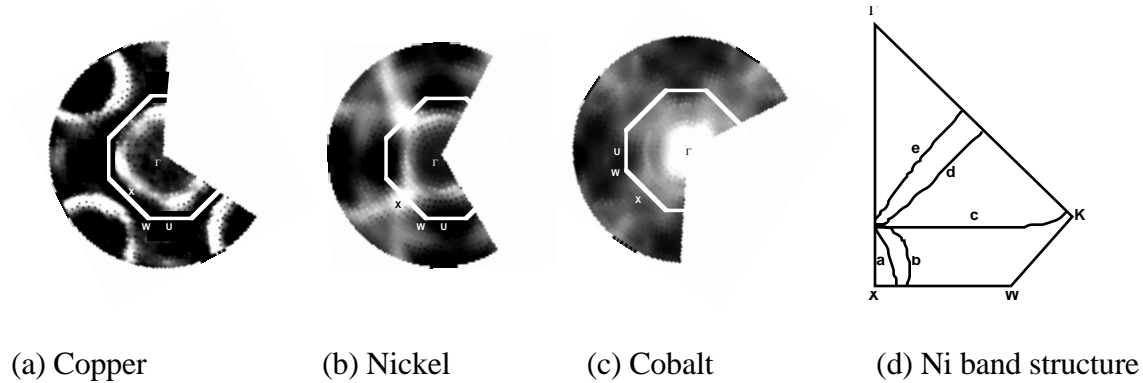


Figure 2. Fermi contour maps taken with a photon energy of $h\nu = 160$ eV of a (a) Cu(100), (b) pure fcc Ni film on Cu(100), and (c) pure fcc Co film on Cu(100), (d) calculated bandstructure at E_F in the (100) plane.

Figure 2 compares Fermi surface photoemission plots from single crystalline Cu (a), and pure fcc films of Ni (b), and Co (c) on Cu(100). All the films have a thickness of 8 ML and the photon energy was fixed at $h\nu = 190$ eV while the angle was varied between 0 and 30° off normal and $\pm 120^\circ$ in the surface plane. At this specific photon energy, a sector of the energy sphere just encloses the (100) plane at the zone boundary, for emission angles smaller than $\pm 20^\circ$. Also shown in Figure 2d is the calculated bandstructure in the (100) plane for Ni [5]. For Cu, contributions from the sp bands on the spherical parts of the Fermi surface are observed, whereas in Ni and Co the d-hole pockets at the X points make an appearance. The sp band feature in Cu begins to shrink

towards the Γ -point, while the d-hole pockets grow around the X-point, in good agreement with the calculated bandstructure.

CONCLUSION

We have measured contour maps of states in momentum space at the Fermi energies of a series of binary alloys of the magnetic transition metals. These alloys possess the same fcc crystallographic structure as that of the Cu(100) substrate when grown as ultrathin epitaxial layers. This implies that the position of the Fermi level is a function of the hole concentration in the d-band, which we vary by alloying the various elements. This is why we expect the Fermi surface contours in k-space to evolve gradually with alloy stoichiometry, greatly aiding identification. We observe sharply defined sp-states throughout k-space characterized by the same ‘dogbone’ structure as that observed in copper. Emptying the d-band leads to states appearing localized in the dogbone region and as a diffuse region at the zone center. Mixing of d- and sp-states, mainly of minority spin polarization, occurs in specific regions of k-space from which derive the “spanning wavevectors” responsible for Fermi surface oscillations and coupling between magnetic layers in spin-valve heterostructures [6]. Future studies will concentrate on these Fermi surface spin-polarized “hotspots”.

ACKNOWLEDGMENT

This work was funded by a grant from the Department of Energy, Office of Basic Energy Science, DOE instrumentation grant # DE-PG02-96er 45595.

REFERENCES

1. F.O. Schumann, S.Z. Wu, G.J. Mankey, and R.F. Willis, Phys. Rev. B, **56**, 2668 (1997).
2. F.O. Schumann, R.F. Willis, K.G. Goodman, and J.G. Tobin, Phys. Lett., **79**, 5166 (1997).
3. J.W. Freeland, I.L. Grigorov, and J.C. Walker, Phys. Rev. B, **57**, 80 (1998).
4. F.J. Himpsel, J.E. Ortega, G.J. Mankey, and R.F. Willis, Adv. in Physics **47**, 511 (1998) and References therein.
5. C.S. Wang and J. Callaway, Phys. Rev. B. **15**, 298 (1977).
6. S.S.P. Parkin, N. Moore, and K.P. Roche, Physical Review Letter, **64**, 2304 (1990).

Principal investigator: Dr. Roy F. Willis, Department of Physics, The Pennsylvania State University. Email: willis@physics.psu.edu. Telephone: 814-865-6101.